Chairman's Message

For all sorts of reasons, last year was something of a turning point for CCP13. John Squire, after forming CCP13 as an SERC initiative some eight years ago, stepped down as Chairman. In his wake he leaves a software initiative that has established an excellent international reputation as a development node for fibre diffraction and non-crystalline diffraction software. It is also one that has had a very clear impact on many biological and non-biological problems. While it is true that CCP13 owes its success to many people, the simple truth is that without John Squire, it would not even exist. We are lucky that John is going to stay heavily involved with CCP13; he remains on the steering committee and also as the editor of *Fibre Diffraction Review*, the CCP13 newsletter that has essentially grown out of its boots and has recently become a refereed journal.

I think that it is also significant that within the last year or so, the full impact of CCP13 activity has started to sink into the wider scientific community. There has always been a large user community in the fibre diffraction/non-crystalline diffraction area. One of the goals of CCP13 was to eliminate the huge duplication of effort that was going on with software and to produce a suite that interfaced well at all levels and indeed where appropriate to other software packages (*e.g.* CCP4). Predictably, the UK community latched on to what was happening with CCP13 quickly, but it is only rather more recently that its impact at an international level has become apparent. Indeed it is gratifying to see CCP13 being reviewed so favourably in mainstream journals such as *Current Opinion in Structural Biology*. With the benefit of hindsight (always nice), it seems easy to see how it has all come together so well:

Firstly, the CCP13 package itself has been extremely well conceived and constructed, mainly as a result of exceptional efforts by Richard Denny, Geoff Mant, and now Mark Shotton. It offers flexible programs that can be applied to a wide range of problems and that are backed with full mathematical rigour. Where appropriate, clear, uncomplicated graphical user interfaces (GUIs) facilitate the use of these programs, making life considerably easier for new users. It is a tribute to the people involved that the CCP13 initiative is, I believe, also on the right track technically. All GUIs are now written in Java and there has been careful evaluation of the relative merits of procedural and object oriented programming for different types of application. In short, CCP13 has its finger on the pulse!

Secondly, to the credit of the steering committee, the project has always had a strong sense of direction. While originally aimed at biological problems involving filamentous molecules (*e.g.* DNA, filamentous viruses, muscle, collagen, cellulose etc.), a decision was made at an early stage to ensure that the software was sufficiently general to apply to non-biological systems and also to disordered polymers and solutions. This is highlighted by the fact that what started off as a purely SERC (biology) and then BBSRC funded activity is now jointly funded by the BBSRC and Daresbury Laboratory, reflecting approximately 50% activity in biological and non-biological areas.

Thirdly, CCP13, together with the Non Crystalline Diffraction (NCD) group at Daresbury, has always attached great importance to the workshops it organises each year, both in terms of the quality of the programme and of the 'hands on' training sessions that have become such a useful feature of the workshop. The first seven of these workshops were held at Daresbury Laboratory but as interest in the project has developed, the possibility of holding these workshops elsewhere arose. Last year the annual workshop was held at St. Andrews University, in honour of Struther Arnott, who has made pivotal contributions to the field of fibre diffraction. By general agreement, the meeting was the best we have ever had and I hope we can continue this trend with the forthcoming meeting at Sheffield University in June 2000.

Lastly, looking through previous copies of the newsletter, I am struck by the steady evolution in the quality of the document and the articles it contains. It started off, as planned, as an informative pamphlet containing useful and relevant information for CCP13 activity. It now exists as a refereed journal, *Fibre Diffraction Review* (ISSN 1463-8401), that in addition to core CCP13/NCD information, contains papers presented at the annual workshop as well as contributed articles. Much of this change is due to the efforts of Geoff Mant and Richard Denny, who have worked very hard on the presentation of the journal. John Squire, as editor, has also over the years consistently pushed the quality of the publication. However, it goes without saying that in

the end, the journal is nothing without your contribution as users. Please remember this for future issues – this is *your* journal and its success will help to ensure continued support of CCP13 from the BBSRC and from Daresbury Laboratory. Whether you are an industrialist, academic staff, or a postgraduate student, please consider submitting articles or reviews of your work to *Fibre Diffraction Review*. We cannot guarantee publication but I know that John will make sure that all articles are refereed well. If it is published, your article will land on the desks of just about everybody in the field.

Please *do* come to the Sheffield meeting in June and please *do* submit your work (whether as a review or otherwise) to *Fibre Diffraction Review*. Please also remember that in addition to the training sessions held at the main annual meeting, CCP13/NCD now runs separate software training workshops for newcomers to the software. Last year the first of these was held at Daresbury Laboratory and was organised by Mark Shotton and Nick Terrill. About 17 people attended and the feedback was very positive. The timing and location of this training workshop makes it an ideal and cheap way for new students to familiarise themselves with the field. If you require any further information on CCP13 and NCD, remember the website at http://www.dl.ac.uk/SRS/CCP13. Also take the few minutes or so that are needed to subscribe to the CCP13 bulletin board (instructions for this at the website).

It just remains for me to thank all those involved for their efforts over the years and to welcome our new steering committee members, Keiichi Namba (Japan), Tom Irving (Illinois, USA), Gerald Stubbs (Vanderbilt, USA), and Rick Millane (Purdue, USA). We are delighted to have their input on the panel.

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Meeting Reports

CanSAS II, 16th May 1999, Brookhaven National Laboratory

On May 16th 1999, a workshop entitled "Data Handling for Small-Angle Scattering" a.k.a. "canSAS II" was held at Brookhaven National Labs as a prelude to the worldwide SAS 99 Congress. The workshop was chaired by John Barnes of NIST, (the chair of the IUCr Commission on Small-Angle Scattering who sponsored the workshop). "canSAS" stands for "Collective Aid to Nomadic Small-Angle Scatterers. "canSAS I" was a workshop in Grenoble in February of 1998 attended mainly by "Instrument Responsibles". canSAS II, in contrast, represented an attempt to bring data handling issues to the larger SAS community which was represented by about 90 attendees.

Wim Bras kicked off the workshop with an overview of the accomplishments of canSAS I and some of the issues raised at the time. More general talks were "Using Statistics to Assess SAS Data Quality" by John Barnes, "Resolution Issues in SAS" by John Barker also of NIST, and "Modeling and Goodness of Fit in SAS Data Reduction" by Jan Skov Pedersen, Risoe. The remainder of the talks and the subsequent panel discussion were aimed directly at the concerns brought out in canSAS I, namely how can we make it easier for users to take home their data and interpret it once they get there? To this end Marc Malfois and Dmitri Svergun from EMBL, Hamburg talked about "sasCIF - A Proposed Standard for 1-D SAS". Joachim Kohlbrecher, PSI, followed up with "One User's Experience with Nexus" which dealt with the Nexus file format, a work in progress which proposes a standard file format for arbitrary SAS data based on HDF. Richard Heenan, of ISIS, followed up with "Existing Tools for SAS Nomads" which was a comprehensive overview of existing programs and their availability.

The remainder of the workshop consisted of a panel discussion moderated by myself (Tom Irving, BioCAT). The main issues that were discussed were:
1) How to make it easier for users to get access to their data.
2) Are we in a position to bless a "standard format" or formats?
3) Can we move towards a "gold standard" software package or packages?